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AN ALGORITHM FOR THE DETERMINATION OF COATING PROPERTIES FROM LASER-GENERATED AND DETECTED RAYLEIGH WAVES USING WAVELET ANALYSIS: APPLICATION TO SPUTTERED TANTALUM

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13. ABSTRACT *(Maximum 200 words)*
We used single-source and single-detector laser-ultrasonic measurements to generate and detect Rayleigh waves on tantalum sputtered steel substrates. Group velocity dispersion curves were calculated from the single-detected signals using wavelet techniques. Theoretical dispersion curves were calculated via the Achenbach and Keshava analysis. A simplex minimization technique between theory and experiment, using known values for the substrate, allowed us to evaluate the coating parameters. The coating thickness was measured accurately with micrometers, and gives the most easily available comparisons with the output of the simplex method. The results using the straightforward wavelet method were compared with an adaptation thereof.

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INTRODUCTION

We are using here the Achenbach and Keshava (ref 1) analysis to calculate dispersion curves and obtain elastic properties of sputtered tantalum coatings. We have previously reported experiments (ref 2), which led to the evaluation of a coating's adhesion. These were based on the analysis of Achenbach and Epstein (ref 3), for the propagation of Rayleigh waves on isotropic coatings. Here we extend our work to obtain elastic properties of sputtered tantalum coatings on steel substrates, based on Achenbach and Keshava (ref 1). The intended use of this effort is for empirical modeling related to wear and erosion, for nondestructive testing (NDT) in-process evaluation of parameters used in deposition processes, and for rapid NDT evaluation of coatings in finished components.

A computer intensive method is used involving a relatively rugged laser-generation and detection system. This consists of a continuous wave laser in a nontemperature or vibration-stabilized Michelson interferometer. Other investigations for obtaining elastic properties and thicknesses of coatings on substrates have been published as follows:

- Ringermacher et al. (ref 4) used Lamb waves
- Schneider et al. (ref 5) used Rayleigh waves with two detectors and obtained phase velocities.

To our knowledge the present work represents the first use of Rayleigh waves, wavelet analysis, and thereby group velocities for coating elastic property determination.

Laser heating causes a pulse of elastic energy in metallic coatings. We generate the surface waves in the thermoelastic regime and use the Cielo et al. (ref 6) annulus technique to obtain a stronger Rayleigh wave signal with no ablation. As the pulse travels along the surface, it spreads as the higher frequencies stay in the coating and the lower ones travel in the substrate. The arrival time of each frequency range reflects the properties of its medium. What starts out as a sharp pulse results in a broadened pulse.

Only one detector is used. The wavelet method enables us to obtain arrival times of the different frequencies contained in the detected pulse. The Achenbach and Keshava (ref 1) analysis for "welded" bonds is used to obtain a 6 x 6 determinant. This is solved numerically to obtain the theoretical dispersion curves (the phase velocity versus frequency), which are a function of the substrate's elastic properties, and also the coating's density, Poisson's ratio, Rayleigh velocity, and thickness.

A simplex algorithm is used to minimize the difference between the dispersion curves obtained from the experiment, with the theory's prediction resulting from the above-mentioned determinant by adjusting the parameters and thickness.

MODEL OF PROPAGATION ALONG A COATED SURFACE AND DISPERSION

Rayleigh waves propagate along the free surface of a semi-infinite solid. Achenbach and Keshava (ref 1) provide a two-dimensional analysis for the "welded" boundary condition for straight-crested free waves in a system consisting of layer (coating) of thickness $2h$ and half space (substrate). The satisfaction of the boundary conditions, obtained using the stress-strain relations and the wave equations, give a determinant whose null solution is a function of the coating and substrate parameters, thickness of the coating, and Rayleigh velocity (refs 1,2). A contour map for the case of tantalum on a steel substrate is shown in Figure 1.

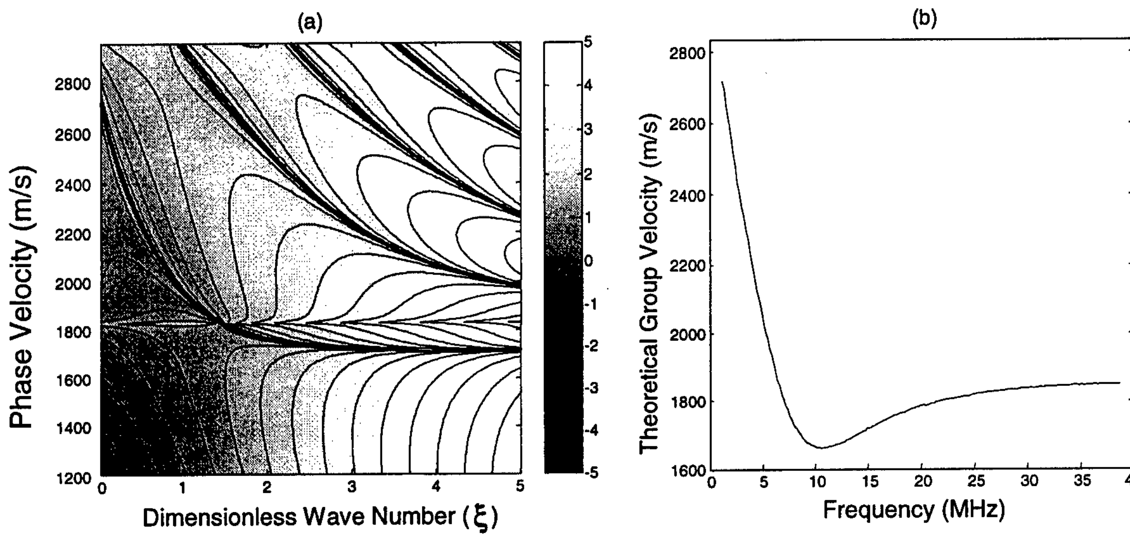

Figure 1. (a) Contour of determinant with phase velocity versus ξ, where $\xi = kh$, k is the wave number, and h is one-half the coating thickness; and (b) theoretical dispersion of a 3-mil (0.003 in.) coating of tantalum on steel.

Instead of using the shear modulus, our input is the Rayleigh velocity V_R for each material. We use the following approximation for the shear velocity V_t. We then obtain the shear modulus (G) as

$$V_t = \frac{V_R(1+\upsilon)}{0.87+1.12\upsilon} \quad and \quad G = \rho V_t^2 \tag{1}$$

THEORETICAL DISPERSION CURVE

Using the outlined theory, we obtain first the phase velocity dispersion, and then the group velocity dispersion. In order to obtain the first mode, we start at high values of ξ. This corresponds to high frequencies where we should only see the effects of the coating. The nondimensional phase velocity in this region should be $V_R(Coating)/V_R(Substrate)$. We take 250 steps through ξ from 5 to 0.1 and utilize the MATLAB *fminbnd* function to find the βs. Allowing for a maximum of 500 iterations, and setting the tolerance limit of β to 10^{-5}, one must be sure that the range of β passed to *fminbnd* straddles the first mode for each value of ξ. Care must be taken when the first mode crosses the point of inflection at $\beta = 0.59$. If too large a range is given, then it is possible for *fminbnd* to return an incorrect value. Once β has been found for all values of ξ, it is multiplied by the shear velocity to obtain phase velocity. The group velocity is computed from $V_g = \delta\omega/\delta k$.

WAVELET APPROACH: DISPERSION CURVES FROM RIDGE OF CONTINUOUS WAVELET TRANSFORM

We utilize a time/frequency continuous wavelet transform method. The signal is converted to the frequency domain using a fast Fourier transform (FFT). The Gabor wavelets in the frequency domain are computed using dyadic scaling, and a bandwidth of 10. Each of these wavelets is multiplied with the FFT of the signal, and transformed back to the time domain using an inverse FFT. A brief theory of the wavelet technique is given below for completeness.

We approximate the ultrasonic signal as a linear combination of harmonic functions, each with a center frequency and given bandwidths. The dispersion relation for group velocities describes the relationship between the frequency f and the velocity v at these center frequencies. For a nondispersive sample, such as an uncoated substrate, the dispersion relation is constant and all the wave components travel with the same phase velocity, which in this case corresponds to the group velocity. The signal thus maintains the same shape as generated. It can be approximated as Gaussian in shape. On this basis we approximate the converging ultrasonic surface wave signal generated by an impulse laser impinging in an annulus as a set of Gaussian signals, each having its own center frequency and its own Gaussian envelope.

$$f(t) = \sum_n a_n e^{-\left(\frac{t-\frac{d}{V_n}}{\beta_n}\right)^2} e^{i\omega_n\left(t-\frac{d}{V_n}\right)} = \sum_n f_n(t) \tag{2}$$

where n is the number of Gaussian packets with amplitude α_n, decay parameter β_n, and center frequency ω_n. The radius of the circular annulus is d and V_n is the group velocity of the packet. For a dispersive, medium V_n is a function of ω_n; d remains the same for all packets.

Consequently, the time of arrival of the various wave components as a function of the frequency can be extracted. Experimentally such dispersion gives the relation between frequency ω_n and group velocity V_n. It depends on the material properties of the coating and substrate, as well as the quality of the bond. Estimation of the dispersion curve is central in determination of parameters using a simplex method. Since each packet is Gaussian, a wavelet transform with a frequency-modulated Gabor mother wavelet, which is also Gaussian, is thought to lead to an optimum correlation.

The continuous wavelet transform of $f(t)$ is defined by

$$Wf(u,s) = \int_{-\infty}^{\infty} f(t) \frac{1}{\sqrt{s}} \psi^{*}\left(\frac{t-u}{s}\right) dt \tag{3}$$

with frequency scaling s and time delay u. The modulated wavelet with a Gabor window is given by

$$\psi(t) = e^{i\eta t} g(t) \tag{4}$$

$$g(t) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha^2}{2}} \tag{5}$$

with center frequency η and variance of $\frac{1}{2\alpha}$. The Fourier transform of the wavelet is given by

$$\hat{\bar{\psi}}(\omega) = \sqrt{s}\hat{\psi}(s\omega) = (4\pi s^2 / \alpha)^{\frac{1}{4}} e^{-\frac{1}{2\alpha}(s\omega - \eta)^2} \tag{6}$$

The bandwidth parameter (BW) discussed above is used to determine α, where $\alpha = 2(\omega_0\, BW/100)^2$.

The wavelet transform can also be expressed as a convolution integral between the signal and the wavelet and its scaled versions.

$$Wf(u,s) = \langle f(t), \psi_{us} \rangle = f * \bar{\psi}_s(u) \tag{7}$$

where

$$\bar{\psi}_s(t) = \frac{1}{\sqrt{s}} \psi^{*}\left(-\frac{t}{s}\right) \tag{8}$$

However, convolution in the time domain is equivalent to multiplication in the frequency domain, hence using the FFT of the signal and the wavelets, the numerical integration is replaced by the dot product of two vectors leading to a fairly fast computation using MATLAB.

If the signal is expressed by a sum of Gaussian packets, as shown in equation (2), the wavelet transform can also be expressed by a sum of wavelet transforms as

$$Wf(u,s) = \sum_n Wf_n(u,s) \tag{9}$$

Substituting the signal from equation (2), it can easily be shown that the wavelet transform consists of two decaying exponentials, one in the time domain and the other in the frequency domain with its maximum value at a single point given by the coordinates

$$u_n = t_n = \frac{d}{v_n} \tag{10}$$

$$\xi_n = \left(\frac{\eta}{s}\right)_n = \omega_n \tag{11}$$

The curve formed by the calculated maxima with coordinates (u_n, ξ_n) is called the ridge of the wavelet transform of the signal, and it represents the group delay versus center frequency of the various signal packets (ref 7). This is the experimental dispersion curve of group delay as a function of frequency.

Once the transform is carried out, the dispersion curve becomes the locus of the ridges of the transform in the frequency-velocity plane.

SIMPLEX METHOD

We estimate various parameters of the layered system by matching the dispersion curve obtained from experiments with that of the theory. This can be done by minimization of the square of the error with respect to several variables. We use the simplex method provided by MATLAB, which returns a local minimum vector *X* near a starting vector *X0*. The procedure uses the Nedler-Mead (direct search) approach.

The objective function is given by

$$F = \sum_{Freq=1}^{M} amplitude(Freq_i)[Disper\_experimental(Freq_i) - Disper\_theory(X)]^2 \tag{12}$$

where the error is the square of the difference between the theoretical dispersion curve and the experimental dispersion curve obtained for each frequency. *X* is the series of parameters used to determine the theoretical dispersion. The set consists of the Rayleigh velocity, density, and Poisson's ratio for the substrate and coating, as well as the thickness of the coating. Any of these parameters can be fixed, depending on the conditions desired. Further, the error is weighted with the amplitude of the spectrum of the experimental signal.

LASER GENERATION AND DETECTION OF SURFACE WAVES

The Nd:YAG laser, with 532-nm wavelength, was used to generate the ultrasonic surface wave along a circle. The other parameters of interest are a 100-mJ energy/pulse and 8 nsec pulse width with a 10 Hz pulse repetition rate. A Michelson interferometer is the means of detection for the surface waves at the center of a generated annulus shown in Figure 2. For an isotropic surface, the waves generated at the annulus all arrive at the center at the same time. In this way, the amplitude of the surface wave is enhanced, resulting in an improved signal-to-noise ratio without ablation. Here we use one-fourth of the annulus for generation. The interferometer is not temperature or vibration stabilized, hence its output has a relatively large amplitude, low frequency sine wave. Superimposed on that is the detection signal due to the Rayleigh wave at the speckle.

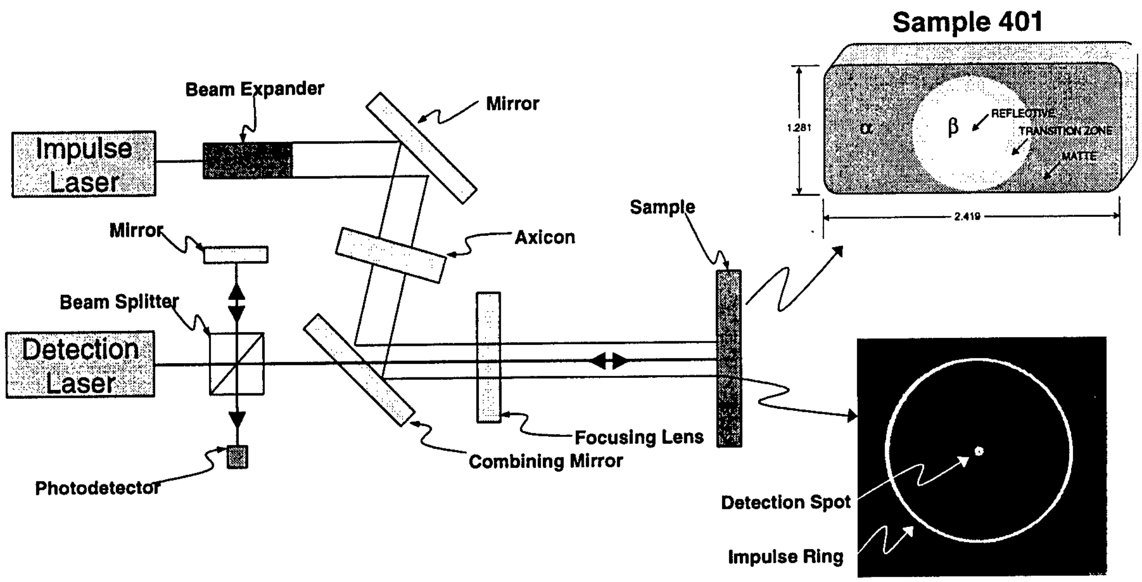

Figure 2. Schematic of Laser-Wave setup, specimen 401,
and image of Zap-It with detector and impulse laser areas shown.

SPECIMENS AND DATA COLLECTION

Two samples were available. They consisted of sputtered tantalum on a steel substrate. Their dimensions in inches were 1.28 x 2.41 x 0.335. The thickness of the coating was not uniform, being thickest at the center. Sputtered tantalum exhibits the alpha body-centered-cubic (bcc) stable phase, and the beta tetragonal unstable phase. One sample (401) had a shiny silvery circle at the center indicating the beta phase, and was a darker matte gray elsewhere, indicating the alpha phase. The other sample (404) was more uniformly shiny tending to indicate that the beta phase was more prevalent, although the edges were more matte. Nothing was done to the samples after sputtering. Each measurement is the average of 300 to 500 traces. The averaging eliminated noise (which is random). All data consisted of at least three sets of measurements.

Measurements were made using the four quadrants of the annulus separately. For the alpha phase in all instances, the thickness was not uniform (but changing linearly with position), but was uniform for the central region of the specimen (beta phase). For uneven thickness over the circle, which constituted the arcs, the thickness of all four arcs was averaged. The micrometer coating thickness was obtained at the center of the circle. Each specimen was measured in three locations: center, upper right corner, and lower left corner. The impulse ring was always one-eighth inch from each edge. This was necessary to eliminate edge effects from showing in the traces.

Data collection was done using LabView. After all the data were collected at a specific point, a piece of "Zap-It" paper was carefully placed on the sample. It was marked by being exposed to the impulse and detector lasers. The detector laser had to be adjusted to a higher intensity for the paper to be affected. In order to determine the distance from each arc to the center of the detection spot, the paper was scanned into a computer using an HP 6300 Scanjet scanner at 1200 dpi. The resulting images were analyzed in Paintshop Pro, where the pixels could easily be counted. On average, the impulse rings were 5 mils wide (6 pixels). The detection spot consisted of two concentric circles. The larger circle had an average diameter of 24 mils and the smaller circle had an average diameter of 8 mils. All distances were measured from the center of the detection spot, to the middle of the impulse ring.

ANALYSIS

The analysis software was written in MATLAB. It begins with obtaining data to be analyzed. Starting values of the thickness, as well as density and Rayleigh velocity, are supplied to the computation. This initial thickness can be estimated from the dip in the nondimensional dispersion curve. Values for the substrate parameters are supplied to the software, as well as the radius of the annulus. Using the wavelet approach, the experimental dispersion curve, Figure 3, is obtained and then matched to the theoretical curve. After convergence is achieved, the system gives the parameters the best fit. The results are given under the heading A in Table 1. The thickness is our check. It was found that the computation gave a thickness that was somewhat underestimated. An arbitrary change was made by comparing the experimental dispersion curve with a function of the theoretical phase and group velocities. The results for both are outlined in the table under the M heading.

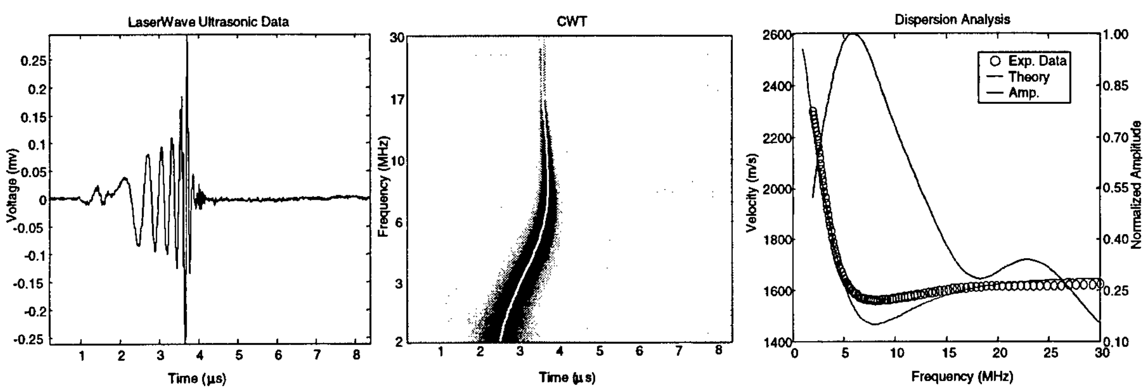

Figure 3. From left to right, the measured signal, the corresponding continuing wavelet transform, and the dispersion.

Table 1. Results

	Thick. (mils)			ρ (g/cm^3)		V_R (m/s)		G (Mbar)		E (Mbar)		V_t (m/s)		V_l (m/s)	
Zone	Meas.	A	M	A	M	A	M	A	M	A	M	A	M	A	M
401 Alpha[1]	3.0	2.7	3.0	17.4	17.8	1711	1722	0.548	0.604	1.480	1.631	1628	1842	3694	3835
401 Alpha[2]	3.6	3.3	4.1	17.9	17.9	1734	1761	0.575	0.635	1.554	1.715	1629	1884	3732	3921
401 Beta	4.9	3.4	4.9	21.5	18.6	1704	1603	0.680	0.547	1.835	1.477	1661	1715	3701	3570
404 Alpha[1]	4.4	3.2	4.1	19.0	18.3	1763	1645	0.640	0.567	1.729	1.530	1704	1760	3821	3663
404 Alpha[2]	4.7	3.6	4.7	18.6	17.8	1749	1623	0.621	0.537	1.676	1.449	1713	1736	3803	3614
404 Beta	6.3	3.6	6.3	27.1	19.1	1687	1601	0.837	0.560	2.261	1.513	1635	1713	3659	3565

1. Measurements taken from the upper right-hand corner of the sample.
2. Measurements taken from the lower left-hand corner of the sample.

DISCUSSION AND CONCLUSION

It is to be noted that the Achenbach and Kashava (ref 1) and Achenbach and Epstein (ref 3) theory for dispersion of the sound velocity on a substrate is based on isotropy of the coating. One feature of such isotropy is that the velocities are equal in all directions. The velocities we measure seem to be equal in the plane of the coating (planar isotropy). With this caution, we compare the thickness values we obtained from the results of this experiment for two techniques. The first is the one described herein, where the theoretical group velocity was used in the simplex method to obtain the relevant parameters. This is labeled as A in Table 1. The other is labeled M and was mentioned above. This averages the dispersion of the group and phase velocities obtained from the theory for use in the simplex method.

The literature seems to estimate that the sputtered beta density (~16.3 to ~17gm/cm^3) can vary, but that for the bcc alpha phase it is ~16.5 (ref 6). We can compare other values obtained as described in this report with literature values for bulk tantalum (nonsputtered alpha) (refs 8,9). We note here the closeness and uniformity of the values for the M method compared to the values of the measured thickness and the reported densities. In all instances, the relative values seem to go toward the tantalum values reported in the literature. The values for Young's modulus and shear modulus also compare favorably with values found in the literature for bulk specimens. Here we note that the 401 alpha visual identification is much more certain than the 404 alpha. The latter was much shinier than the former. In addition, even though both specimens were sputtered under identical conditions, the time for sputtering was ~50% greater for 404. At the moment, we note that the match between the micrometer measurements and those of the M method is quite good. Measurements for the A method are 0.0012 inch on average. The latter is a 26% difference for an average coating thickness of 0.0045 inch for both phases. The density difference between the M results and the 16.6 g/cm^3 is 8%; the density difference for the A results is 10%. The computed shear and longitudinal velocities as indicated here are also compared. The values of E, G, and the velocities are approximations based on the values obtained here.

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